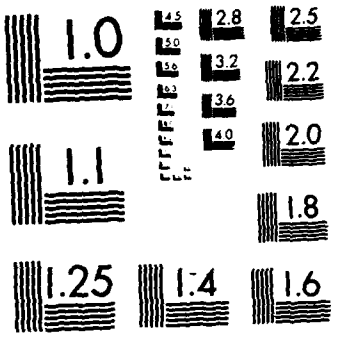
AD-A143 426 THEORY OF THE ELECTRONIC PROPERTIES OF MERCURY-CADMIUM-TELLURIDE ALLOYS(U) AUBURN UNIV AL A B CHEN ET AL. 21 FEB 84 AFOSR-TR-84-0549 1/1

UNCLASSIFIED F49620-81-K-0012 F/G 20/12 NL

END

FILMED

DTIC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

(10)

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER [redacted] 19
2. GOVT ACCESSION NO
3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle)
Theory of the Electronic Properties of Mercury-Cadmium-Telluride Alloys

5. TYPE OF REPORT & PERIOD COVERED
Final Report
(81-6-31 to 83-12-31)

6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s)
An-Ban Chen and
Arden Sher (SRI International)

8. CONTRACT OR GRANT NUMBER(s)
F49620-81-K-0012

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Auburn University
202 Samford Hall
Auburn, AL 36849

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
2306/C2 61102F

11. CONTROLLING OFFICE NAME AND ADDRESS
Directorate of Electronic & Material Science
AFOSR/NE, Building 410
Bolling, AFB, DC 20332

12. REPORT DATE
84-2-21

13. NUMBER OF PAGES
7

14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)

15. SECURITY CLASS. (of this report)
Unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release;
distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)
Mercury-Cadmium-Telluride Alloy, Band Structure, Disorder, Density of States
Structural Properties, Band Gap, Vacancy, Dislocation, Infrared Material

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

See reverse side.

DTIC ELECTE JUL 27 1984 S D

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

ABSTRACT

An accurate band-structure theory for semiconductor alloys was achieved. It has been successfully applied to Mercury-Cadmium-Telluride alloys (MCT), and is being extended to III-V and other II-VI semiconductor alloys. As a result of this research, ten papers have been published. Several other papers and one book are in progress. The most important finding was the origin of the major disorder and its effects on different parts of the band structure. The large s-energy fluctuation between the Hg and Cd sites was found to cause a large smearing in the density of states about 5 eV below the top of the valence band, but it produced very little bowing and scattering for the states near the band gap. A detailed study of these facts accounts for the lattice instability of MCT and its very high electron mobility. Another significant result is that, while Cd weakens a neighboring Hg-Te bond, Zn strengthens it. This helps to explain the ease of Hg vacancy formation in HgCdTe alloys, and predicts that Hg vacancies should be less of a problem in HgZnTe. Moreover we have demonstrated that dislocation energies in semiconductors are proportional to the reciprocal of the ninth power of the near neighbor bond length. This explains why a small percentage of Zn added to the CdTe substrates greatly reduces the dislocation density. Such structural studies may help resolve the adverse structural difficulties affecting MCT as an infrared material.

I. STATEMENT OF WORK AND SIGNIFICANT ACHIEVEMENTS

Auburn University and SRI International have performed the following tasks for a cooperative research on the electronic properties of Mercury Cadmium Telluride alloys:

(1) Incorporate relativistic interactions into the existing theory.

(2) Increase the basis set to include d-states.

(3) Derive a CPA generalization to the Brooks mobility formula.

(4) Compare the resulting band theory to experiment.

(5) Add temperature variations.

(6) Calculate the Auger recombination rate.

(7) Calculate full transport and optical properties.

(8) Calculate the energies of impurity states and vacancies.

(9) Calculate the free energy of impurities and vacancies.

(10) Add effects of reconstruction to Tasks 8 and 9.

(11) Calculate the electronic structure and configuration of surfaces.

(12) Calculate interface states with insulators.

Our objective to devise an accurate band-structure theory for semiconductor alloys has been achieved. The theory has been successfully applid to HgCdTe alloys and is being extended to III-V and other II-VI semiconductor alloys. Ten papers from this research have been published and several more are in progress. As a result, we are writing a book entitled Semiconductor Alloys to be included in the new Plenum series of books on Microelectronics Physics and Fabrication.

Our most important finding is the understanding of the origin of the major alloy disorder in HgCdTe and its affects on different parts of the band structure. The largest disorder was found to be the s-energy variation between the Hg and Cd sites due relativistic effects. This s-energy fluctuation causes a large semearing in the density of states about 5 eV below the valence band top, but only produces a small bowing and scattering for the states near the band gap. This result was confirmed by a recent photoemission study by Spicer's group and is consistent with the high electron mobility found in this material.

Another significant result has come from our recent structural studies. We found that while Cd weakens a neighboring Hg-Te bond, Zn strengthens it. This is significant because experiments in SBRC demonstrated that the dislocations of HgCdTe alloys grown on ZnCdTe substate were at least one order magnitude less than those grown on CdTe substate. The continuation of this structure study bears some promise to help resolve the adverse structural problems affecting the utility of HgCdTe as an infrared material.

II. PUBLICATIONS

1. CPA Band Calculation for (Hg,Cd)Te, A.-B. Chen and A. Sher, J. of Vacuum Science and Technology 21 (1), 138-144 (1982).

2. Cation Bond in $Hg_{1-x}Cd_xTe$, J.A. Siberman, P. Morgan, W.E. Spicer, A.-B. Chen, A. Sher and J.A. Wilson, J. of Vacuum Science and Technology (Sept/October Issue, 1982).

3. Dominance of Atomic States in a Solid: Selective Breakdown of the Virtual Crystal Approximation in a Semiconductor Alloy - $Hg_{1-x}Cd_xTe$, W.E. Spicer, J.A. Siberman, P. Morgan, I. Lindau, J.A. Wilson, A.-B. Chen, and A. Sher, Phys. Rev. Letters 47, 948-951 (1982).

4. Unusual Behavior of $Hg_{1-x}Cd_xTe$ and Its Explanation, W.E. Spicer, J.A. Siberman, P. Morgan, I. Lindau, J.A. Wilson, A.-B. Chen, and A. Sher, Physica 117B4118B, 60 (1983).

5. Construction of Orthonormal Local Orbitals and Application to Zinc-blende Semiconductors, A.-B. Chen, and A. Sher, Physical Review B26, 6603, (1982).

6. Calculation of Optical Properties of Semiconductors with the Use of Simple Orbitals, A.-B. Chen, S. Phokachaipatana, and A. Sher, Phys. Rev. B. 28, 1211 (1983).

7. Relation Between the Electronic States and Structural Properties of $Hg_{1-x}Cd_xTe$, A.-B. Chen, A. Sher, and W.E. Spicer, J. of Vac. Sci. & Technol. A1 (3) 1674 (1983).

8. Band Gap Variations and Lattice, Surface and Interface Instability in $Hg_{1-x}Cd_xTe$ an Related Compounds, W.E. Spicer, J.A. Silberman, I. Lindau, A.-B. Chen, and A. Sher, J. Vac. Sci. & Technol. A1 (3), 1735 (1983).

9. On the Determination of the Energy Band Offsets in $Hg_{1-x}Cd_xTe$ Heterojunctions, T.N. Casselman, A. Sher, W.E. Spicer, and A.-B. Chen, J. Vac. Sci. & Technol. A1 (3), 1692 (1983).

10. Dislocations in HgZnTe and HgCdTe Alloys, A. Sher, A.-B. Chen, and W.E. Spicer, in preparation for publication in Appl. Phys. Lett.

11. Bond Length and Bond Energy Modification in Alloys, A. Sher, A.-B. Chen, W.E. Spicer, and Ken Shih, in preparation for publication in Appl. Phys. Lett.

12. Sensitivity of Defect Levels to Band Structures and Impurity Potentials in CdTe, HgTe and HgCdTe Alloys, A.-B. Chen and A. Sher, in preparation for pub. in Phys. Rev. B.

13. Semiconductor Alloy, A.-B. Chen and A. Sher, Microscience (SRI International Multiclient Study) Issue 4, 179-250 (1983).

III. RESEARCH PERSONNEL

Auburn University:

An-Ban Chen, Professor

P.C. Sharma, Postdoctoral Research Associate

S. Phokachaipatana, Graduate Research Assistant
Master Thesis: "Calculation of Optical Properties of Semiconductors Using Simple Orbitals" (Completed Dec., 1982)

J. Cherng, Graduatte Research Assistant
Master Thesis: "Vacancy State in Hg Te, CdTe and Their Alloys" (In Progress)

K. Clements, Graduate Research Assistant

SRI Inernational:

Arden Sher, Staff Scientist

IV. INTERACTIONS

A. Papers presented at meetings:

1. "Cation Bond in $Hg_{1-x}Cd_xTe$" J.A. Siberman, P. Morgan, W.E. Spicer, A.-B. Chen, A. Sher, and J.A. Wilson, presented at the Ninth Annual PCSI Conference: Physics and Chemistry of Semiconductor Interfaces, Pacific Grove, California, 27-29 January 1982.

2. "Orthogonalized local Basis for Zinc-Blende Semiconductors" A.-B. Chen and A. Sher, Dallas meeting of the American Physical Society, 8-12 March 1982.

3. "Calculation of Optical Properties of Semiconductors Using Simple Orbitals" S. Phokachaipatant and A.-B. Chen, Dallas Meeting of the American Physical Society, 8-12 March 1982.

4. "CPA Calculation of the HgCdTe Band Structure" A. Sher, HgCdTe DARPA Program Review, Stanford University, Spring 1982.

5. Properties of Surfaces, Near Surface Regions, and Interfaces of MCT Materials and Structures, J. Wilson, W.E. Spicer, A. Sher, R. Wilson, 3rd Annual Review of Defense Advanced Research Projects Agency, Defense Sciences Office, Focal Plane Materials Research Program.

6. Relation Between the Electronic States and Structural Properties of $Hg_{1-x}Cd_xTe$, A.-B. Chen, A. Sher, W.E. Spicer, the 1983 U.S. Workshop on the Physics and Chemistry of Mercury Cadmium Telluride, Feb. 8,9,10 1983, Dallas, Texas.

7. $Hg_{1-x}Cd_xTe$ Surfaces, Interface, Bulk Defects and Movement of Defects, W.E. Spicer, J.A. Silberman, I. Lindau, J.A. Wilson, A. Sher, A.-B. Chen, ibid.

8. On the Determination of the Energy-Band Offset in $Hg_{1-x}Cd_xTe$ Heterojunctions, T.N. Casselman, A.-B. Chen, A. Sher, J.A. Silberman and W.E. Spicer, Ibid.

9. Electron Properties of HgCdTe Alloys and Deep States in CdTe, A. Sher, A.-B. Chen, W.E. Spicer, J. A. Silberman "CdTe-HgCdTe Workshop" SERI, Golden Co. January 5, 1984.

10. Characterization and Passivation of HgCdTe Surfaces, J. Wilson, W.E. Spicer, J.A. Silberman, A. Sher, R. Wilson DARPA/DSO Contractor Program Review Local Plane Array Materials, Processing and Device Research, 6-7 February 1984.

B. Seminars

"Calculate Band Structures for HgCdTe Alloys", by An-Ban Chen at Santa Barbara Research Center, May, 1983.

"Electronic Structure of Semiconductor Alloys", by An-Ban Chen at Auburn University, Nov., 1982 and at NASA Space Flight Center in Huntsville, January, 1984.

"Structure Properties of Semiconductor Alloys", by Arden Sher at Auburn University, Feb., 1984; and at Stanford University, Feb., 1984.

C. Interactions With Other Groups

We have a close working relationship with the experimental group headed by W.E. Spicer at Stanford University. This interaction has been extremely fruitful. We are also working with W.A. Harrison (Applied Physics) with F. Gibbons (Electrical Engineering) and with D. Stevenson (Materials Science), all at Stanford. Another interaction has been established with the HgCdTe research group at SBRC. Some initial contact has also been made with R.D. Graft at the Army Night Vision and Optical Electronics Laboratory and with the HgCdTe group at the NASA Space Science Laboratory in Huntsville.

V. PATENT: None